Tetradeca-1,13-diene

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 1.87e-08 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.81e-01

Confidence level: 4.78e-01

Nearest Neighbors from the Training Set

Image not found
Tridecane
Measured: 2.55e-08
Predicted: 1.55e-08

Image not found
Tetradecane
Measured: 1.97e-08
Predicted: 1.05e-08

Image not found
Undecane
Measured: 2.82e-08
Predicted: 1.58e-07

Image not found
Pentadecane
Measured: 3.58e-10
Predicted: 1.53e-09

Image not found
Benzene, octyl-
Measured: 3.47e-07
Predicted: 1.23e-06